

Book Reviews

ACS Symposium series 589

Computer-aided molecular design. Applications in agrochemicals, materials and pharmaceuticals, ed. Charles H. Reynolds, M. Katharine Holloway & Harold K. Cox, American Chemical Society, Washington DC, 1995, x + 428 pages, price US\$109.95. ISBN 0-8412-3160-5

This book reports on a symposium held as part of the 207th national meeting of the American Chemical Society, San Diego, March 1994. The aim of the symposium series is to provide a rapid means of publication and, given that these papers are peer reviewed, this appears to have been achieved for this volume. The contents are evenly divided between agrochemicals, materials and pharmaceuticals and thus about one-third of the volume will be directly relevant to a researcher involved in one of these fields. Some of the topics, however, are of more general interest, for example the effect of tautomeric equilibria on hydrophobicity (A. J. Leo), experimental design in organic synthesis (L. H. Brannigan *et al.*), the use of predictive toxicology in the design of new chemicals (V. K. Gombar and K. Enslein) and the use of genetic algorithms in computer-aided molecular design (V. Venkatasubramanian *et al.*). Other papers which present an example from a particular field contain sufficient information to provide a useful practical guide to particular computational techniques. As a result this volume should be of interest to many who may use computer-aided molecular design (CAMD), whatever their field of work.

The methodology covered in this book is very varied including 'classical' QSAR using regression analysis, 3-D QSAR (CoMFA and HASL), semi-empirical and *ab initio* quantum mechanics calculations, molecular dynamics simulations, multivariate statistics, expert systems and genetic algorithms. The examples are similarly varied and cover theoretical studies of explosives and corrosion, modelling drug diffusion in membranes, the inclusion of metabolism and toxicology in design and the simultaneous analysis of in-vivo and in-vitro data. In the preface the editors highlight a commonly posed question about computer-aided molecular design—'What new products have arisen as a result of CAMD?'. It may be argued that this is not really a

question since the same query is never made about the utility of other tools such as NMR and crystallography. There are, however, sufficient examples shown here to answer this question successfully. One in particular, which illustrates the use of a genetic algorithm for the selection of Human rhinovirus serotypes for compound testing (Jaeger *et al.*), specifically demonstrates the impact of CAMD on the project team.

As the series editor points out in the foreword a book such as this can only provide a 'snapshot in time' of the current state of research on a topic. Some of the techniques described here will have moved on since 1994, particularly the more recent artificial intelligence methods, but the applications of the techniques provide sound examples of the practical use of CAMD. A 'proceedings' volume is always useful to someone who might have attended a conference but was unable to. In the case of this book I have no hesitation in recommending it both to the specialists who apply and develop computer-aided molecular design techniques and to the experimentalists who seek to make use of the methods in their work. These were the two audiences that the editors of this volume had in mind, for both the symposium and the book, and I feel that they have met their target admirably.

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Biorational pest control agents—Formulation and delivery, ed. F. R. Hall & J. W. Barry, American Chemical Society, Washington DC, 1995, xii + 306 pp., price US\$84.95.

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The aim in the United States of implementing integrated pest management (IPM) on 75% of all agricultural lands by the year 2000 is linked with the aim of reducing pesticide use and of using safer pesticides. In view of these aims, the American Chemical Society sponsored a Symposium on Formulation and Delivery of Biorationals in March 1994. This book provides a wider audience with the papers discussed at the symposium. While many non-conventional pesticide control